Transient deterministic modeling of neutral gas flow in DEMO particle exhaust system

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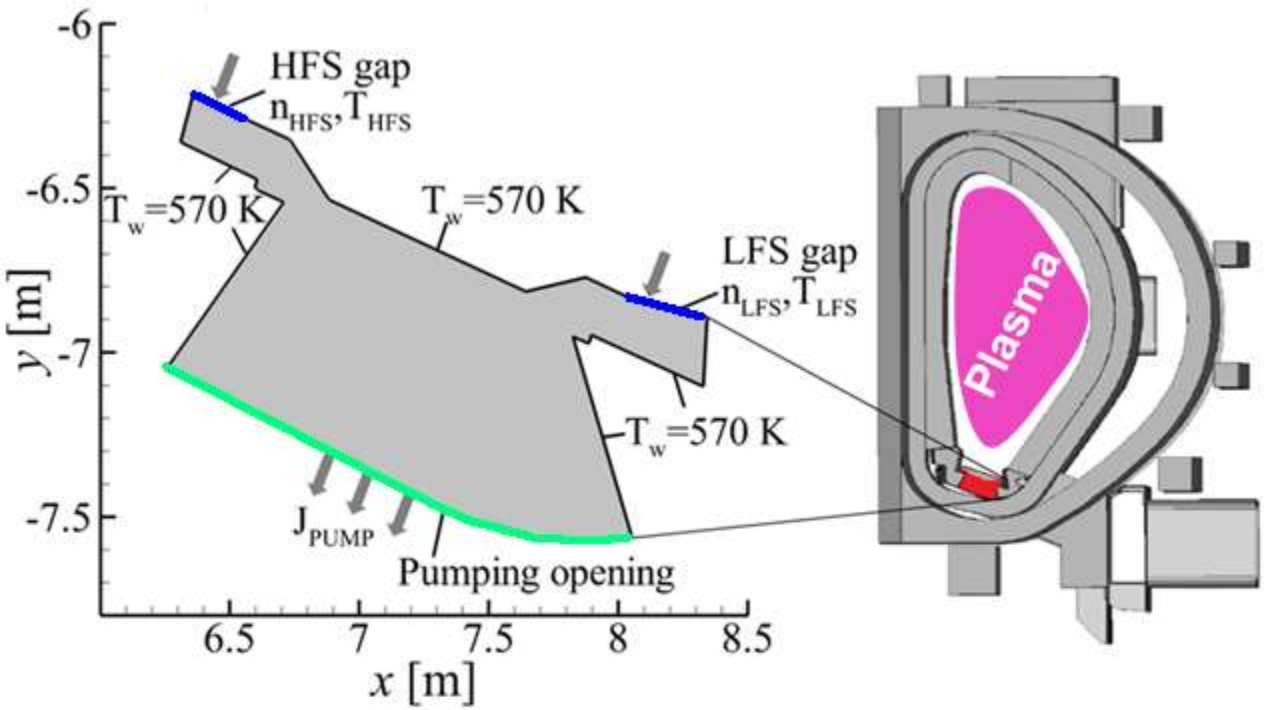
Scope & Motivation

- Over the last few years much effort has been invested in the modeling of the complex particle exhaust systems of fusion reactors operating in a wide range of the Knudsen number from continuum and slip flow regime, until transitional and even free molecular regime
- The rarefied flow behavior in these systems cannot be properly captured by the typical Navier-Stokes-Fourier approach and must be described by the integro-differential Boltzmann equation, the DSMC (Direct Simulation Monte Carlo) method or the DVM (Discrete Velocity method) method
- The main drawback of the DSMC method is the long time averaging of the macroscopic quantities needed in order to avoid statistically noisy results – Extremely time consuming in the transient studies
- The appropriate estimation of the transient response behavior of the particle exhaust system in fusion reactors is very important in all relevant modelling activities concerning plasma scenario optimization and divertor development
- In the present work, the well-established DVM method is applied to predict the transient behavior of the neutral gas flow in the particle exhaust system of **DEMO** (**DEMO**nstration Fusion Power Plant) fusion reactor

DEMO divertor flow set-up



- Boundary conditions (typical operational detached plasma scenario of DEMO):

n_{HFS} [m^{-3}]	n_{LFS} [m^{-3}]
13.28×10^{19}	13.28×10^{19}

T_{HFS} [K]	T_{LFS} [K]
4000	4000

- The problem of neutral gas flows inside the pumping area of the DEMO nuclear fusion reactor is considered

- The transient behavior of the D_2 neutral gas flow is modeled assuming various initial pressure conditions scenarios from 0.01 Pa up to 1 Pa (Transient plasma data is currently not available)

- Various values of the capture coefficient ξ at the pumping port are assumed ($0.02 \leq \xi \leq 0.3$)

DVM method

- The complicated collision term of the Boltzmann equation is replaced by kinetic models

$$\frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f = \Omega_{collisions} \Rightarrow \frac{\partial f}{\partial t} + \boldsymbol{\xi} \cdot \nabla f = \frac{nkT}{\mu}\left[f^{\mathrm{model}} - f \right], \quad f\left(\boldsymbol{r},\boldsymbol{\xi},\boldsymbol{t}\right)$$

- In the DVM method the continuum spectrum of magnitudes of the molecular velocity is replaced by a set of discrete magnitudes ξ_α

$$\frac{\partial f_a}{\partial t} + \boldsymbol{\xi}_a \cdot \nabla f_a = \frac{nkT}{\mu}\left[f_a^{\mathrm{model}} - f_a \right]$$

- The Shakhov kinetic model is used (Excellent agreement with the BE, correct Prandtl number, good choice for coupled flow and heat transfer phenomena):

$$f^{\mathrm{model}} = \frac{nm^{3/2}}{\left(2\pi kT\right)^{3/2}} \exp\left[-\frac{m\left(\boldsymbol{\xi} - \boldsymbol{u}\right)^2}{2kT} \right] \left\{ 1 + \frac{(1-\mathrm{Pr})m\left(\boldsymbol{\xi} - \boldsymbol{u}\right)\cdot \boldsymbol{q}}{5nk^3T^3} \left[\frac{m\left(\boldsymbol{\xi} - \boldsymbol{u}\right)^2}{kT} - 5 \right] \right\}$$

- The effect of the intermolecular potential is inserted via the choice of the viscosity coefficient (VHS model)

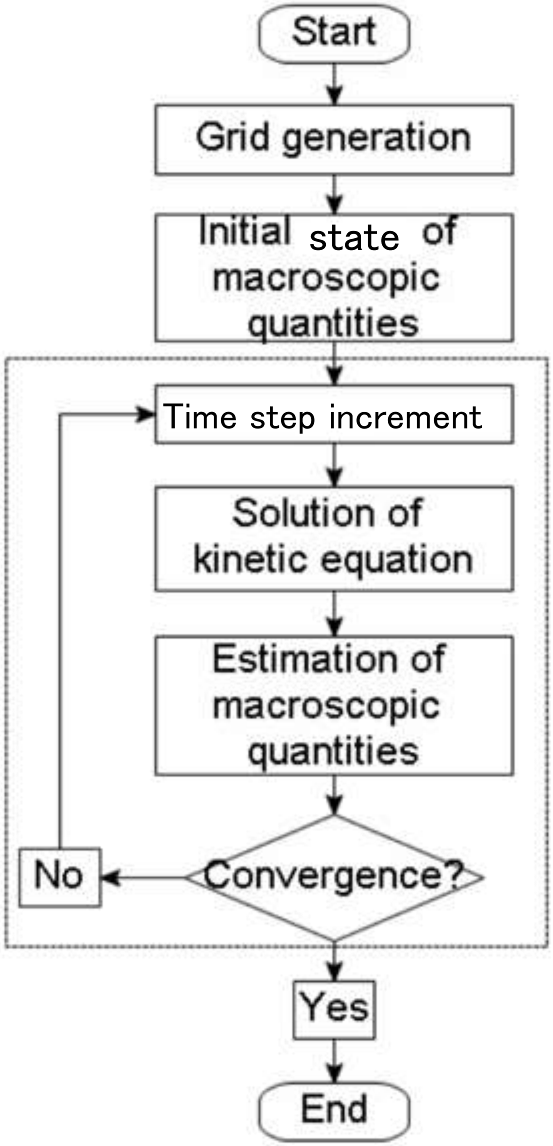
$$\mu = \mu_0 \left(T / T_0 \right)^{\omega}$$

- The value of 0.5 corresponds to the case of Hard-Sphere potential, while a value between 0.5 and 1 is expected for real gases (0.74 in the case of D_2)

Deterministic algorithm

- A uniform/non-uniform grid is applied in the physical space
- In the molecular velocity, the DVM method is applied
- The solution algorithm consists of the following steps:
  1. Initialization of macroscopic quantities
  2. Solution of governing equation
  3. Estimation of macroscopic quantities

  Steps 2-3 are repeated at each time step until the relative change in macroscopic quantities between two iterations is less than 10^{-8}
- The velocity space has been discretized using 28x28 velocities and in the physical space a triangular mesh of 30000 elements has been used
- The code was recently validated by performing comparison against DSMC simulations [1]

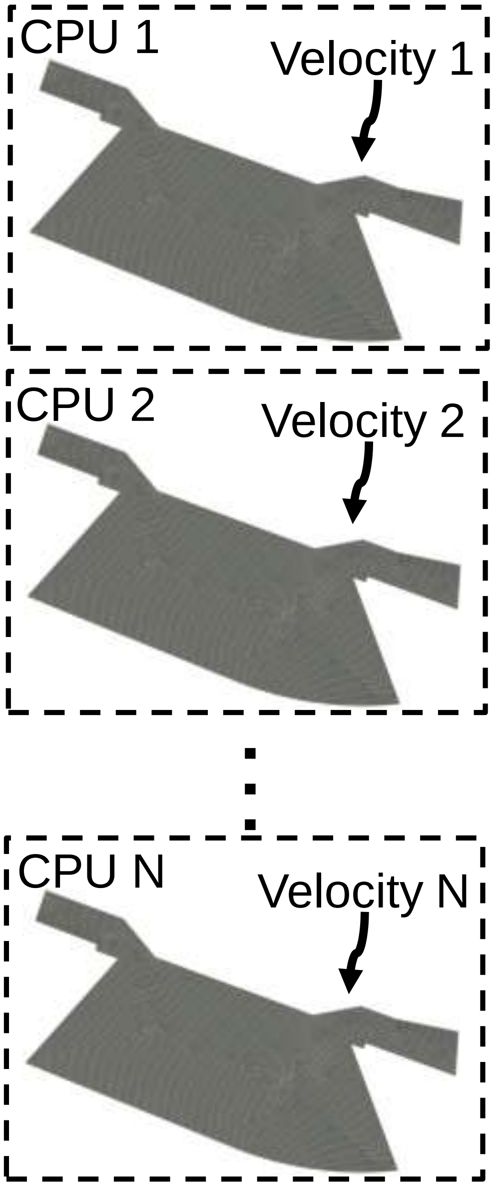


[1] *C. Tantos et al., 10.1116/6.0000491*

Parallelization strategies: VSD

Velocity Space Decomposition (VSD)

- Basic idea: each CPU is assigned a velocity from the velocity space but solves for all nodes of the physical space
- The communication only takes place when evaluating the moments – and then each core will get the complete information for the moments (MPI_Allreduce)
- VSD can be very easily implemented and has been proven to be a very robust and efficient strategy [1,2]
- For the very large number of cells the transferred message for the evaluation of the macroscopic quantities becomes large
- Global reductions using a large number of MPI processes also lead to a decrease in the parallel efficiency because they are natural barriers between computations



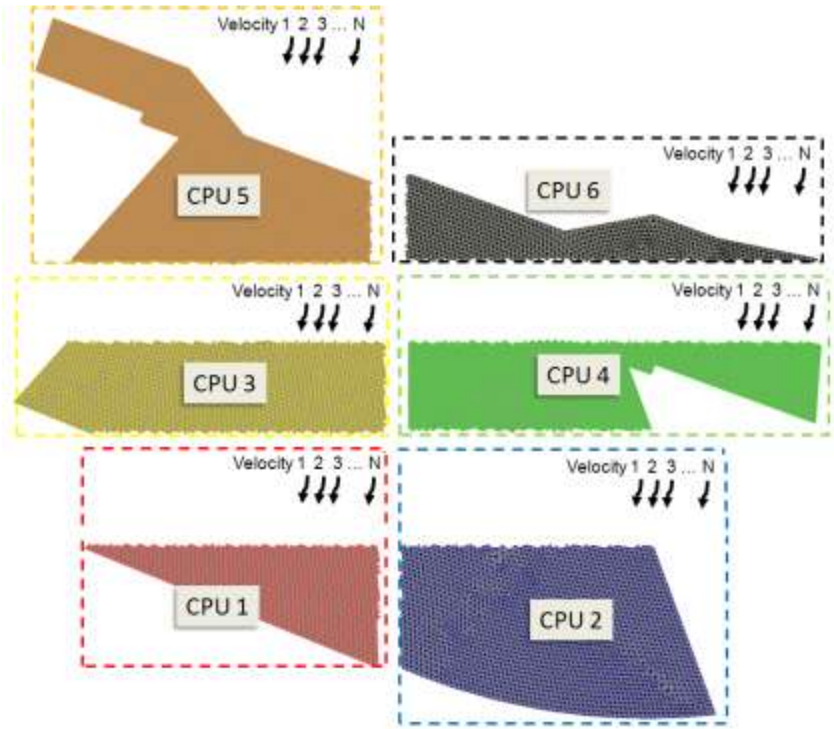
[2] *C. Tantos, 10.12681/eadd/37406;* [3] *S. Pantazis, 10.12681/eadd/24649*

Parallelization strategies: PSD

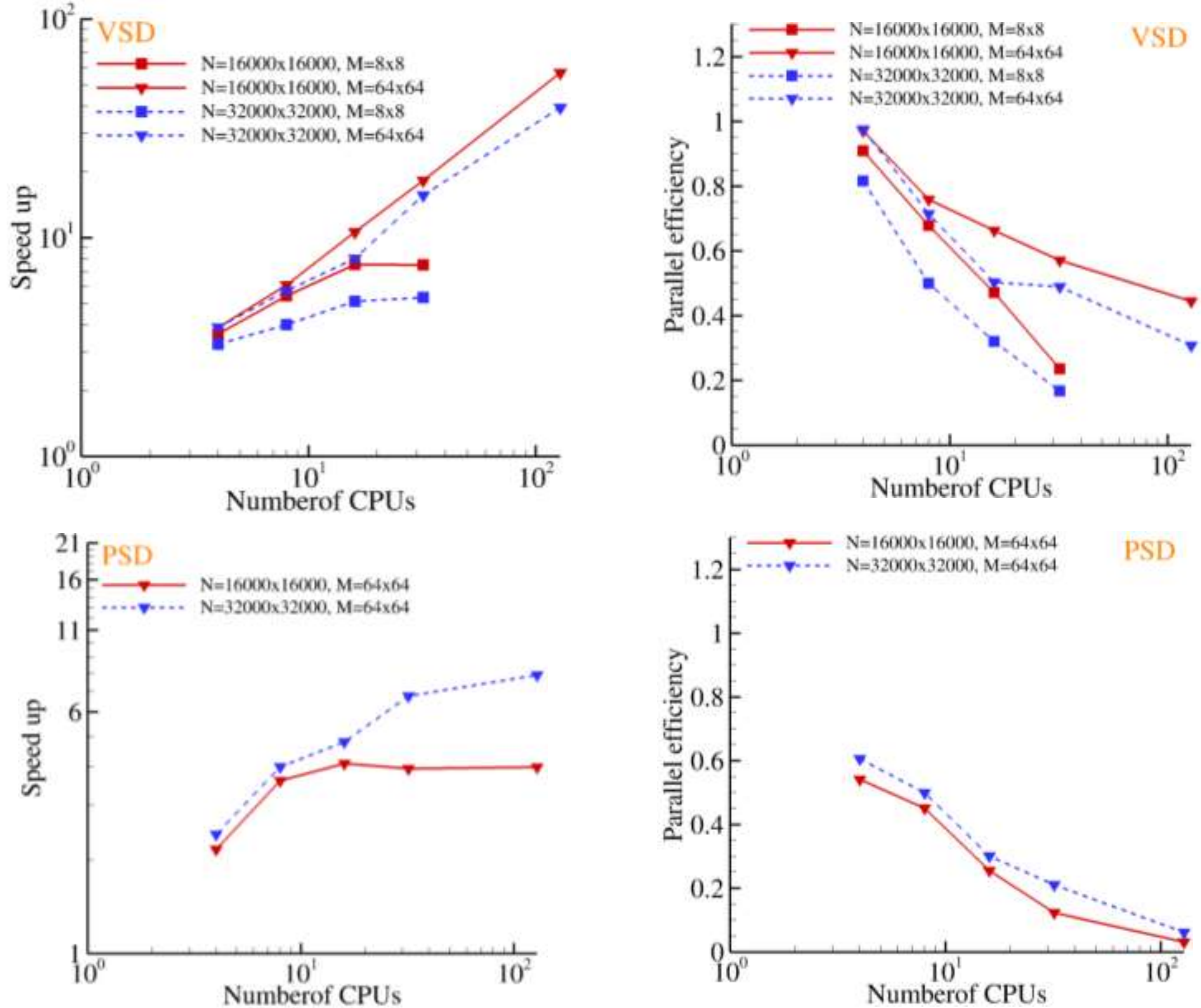
Physical Space Decomposition (PSD)

- Basic idea: each CPU is assigned a sub-domain of the whole physical domain but solves for all nodes of the velocity space
- The halo layer concept to account for the communication between the sub-domains is applied
- Halo layer covers all processor boundaries and is explicitly updated through parallel communication calls
- For very large number of discrete velocities, the communication network will be overloaded by a large number of small messages
- The parallel efficiency of the PSD strategy is expected to be lower compared to the VSD approach (in highly non-equilibrium flows)

PSD example using 6 CPU cores

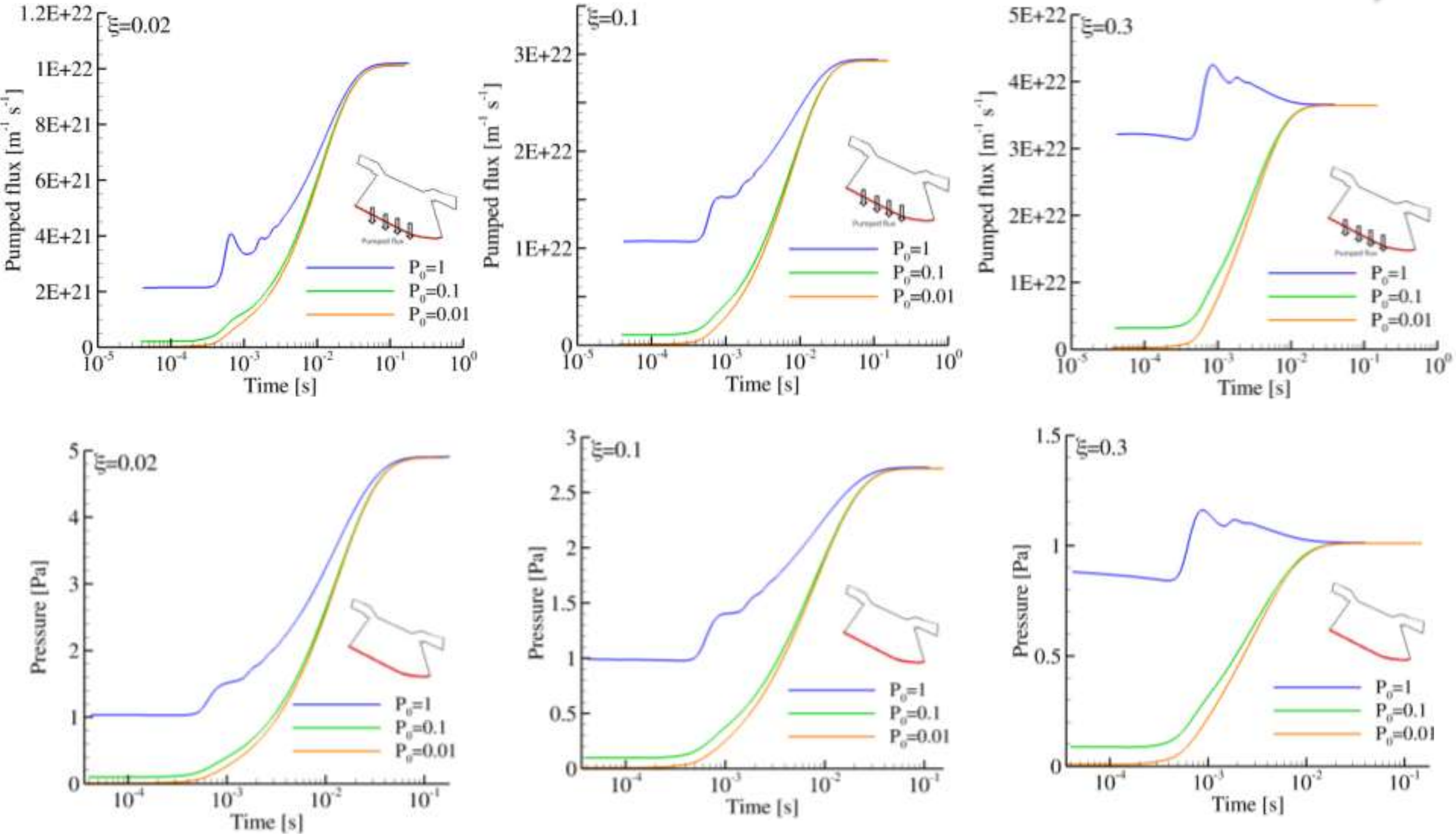


Speed up & Parallel efficiency

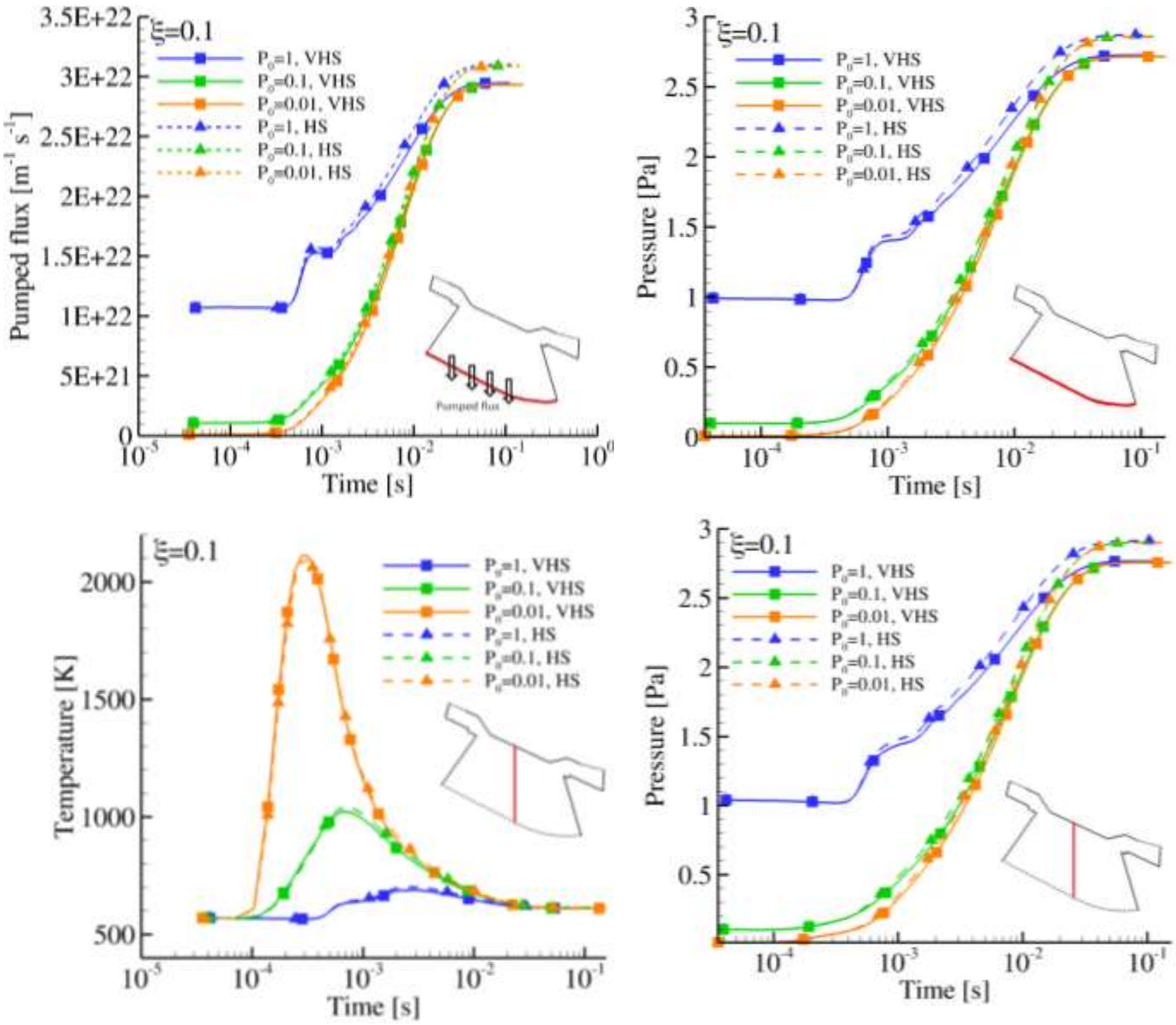


Pumped flux & Pressure @ port vs time

Pumping intensity (ξ)



Effect of intermolecular potential model



Key points summary

- An initial study of the transient behavior of the neutral gas flow inside the DEMO (DEMOnstration Fusion Power Plant) particle exhaust system has been performed in a wide range of the operating conditions
- The results show, that the applied deterministic methodology allows a computationally efficient transient study of the neutral gas dynamics in the particle exhaust of the fusion reactors, using nowadays High Performance Computing (HPC) centers
- The divertor was found to have typical reaction times of 0.1 sec
- For the low initial pressure scenario the evolution of the pumped flux follows a smooth behavior, while for the high initial pressure scenario oscillations are observed
- The intermolecular potential does not affect the transient behavior of the particle exhaust system – the pumped flux is slightly affected, about 5%
- The current study is planned to be extended in the case of 3D flow set-ups as well as using the transient boundary conditions, as soon as they become available

thank you!